INFRARED SPECTRA OF PROTONATED AROMATIC HYDROCARBONS AND THEIR NEUTRAL COUNTERPARTS IN SOLID $PARA$-HYDROGEN

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Protonated polycyclic aromatic hydrocarbons (H^+PAH) have been reported to have infrared (IR) bands at wavenumbers near those of unidentified infrared (UIR) emission bands from interstellar objects. However, recording IR spectra of H^+PAH in laboratories is challenging. Two spectral methods have been employed previously to yield IR spectra of H^+PAH. One employs IR multiphoton dissociation (IRMPD) of H^+PAH, but the bands are broad and red-shifted. [a] Another measures the single-photon IR photodissociation action spectrum of cold H^+PAH tagged with a weakly bound ligand, such as Ar, but application of this method to large PAH is difficult.[b] A new method for investigating IR spectra of H^+PAH and their neutral counterparts was developed using electron bombardment during p-H_2 matrix deposition. With this technique, we have recorded IR absorption spectra of protonated forms of benzene ($C_6H_7{}^+$), naphthalene (1- and 2-$C_{10}H_9{}^+$), pyrene (1-$C_{16}H_{11}{}^+$), coronene (1-$C_{24}H_{13}{}^+$), and their neutrals.[c] The significant superiority of the spectra thus recorded to those with the Ar-tagging and IRMPD methods is demonstrated. The narrow widths of the lines enabled us to distinguish clearly between isomers 1-$C_{10}H_9{}^+$ and 2-$C_{10}H_9{}^+$; 2-$C_{10}H_9{}^+$ was unstable and converted to 1-$C_{10}H_9{}^+$ in less than 30 min. A survey of these experimental results shows that three major lines in the 7-9 μm region are red-shifted from 7.19, 7.45, and 8.13 μm of 1-$C_{16}H_{11}{}^+$ to 7.37, 7.53, and 8.21 μm of 1-$C_{24}H_{13}{}^+$, showing the direction towards the UIR bands near 7.6, 7.8, and 8.6 μm. In contrast, the line at 11.5 μm for 1-$C_{16}H_{11}{}^+$ is blue-shifted to 11.4 μm for 1-$C_{24}H_{13}{}^+$, showing the direction toward the UIR band near 11.2 μm. Other examples will be presented if time permits.

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[a] O. Dopfer, *PAHs and the Universe,* **46**, 103 (2011).

[b] A. M. Ricks, G. E. Douberly, M. A. Duncan, *Astrophys. J.* **702**, 301 (2009).

[c] M. Bahou, Y.-J. Wu, Y.-P. Lee, *J. Chem. Phys.* **136**, 154304 (2012); M. Bahou, Y.-J. Wu, Y.-P. Lee, *Phys. Chem. Chem. Phys.* **15**, 1907 (2013); M. Bahou, Y.-J. Wu, Y.-P. Lee, *J. Phys. Chem. Lett.* **4**, 1989 (2013); M. Bahou, Y.-J. Wu, Y.-P. Lee, *Angew. Chem. Int. Ed.* **53**, 1021 (2014).